=> d 12; d his; log y L2 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation. L2 QUE  $\overrightarrow{ABB}=ON$  PLU=ON L1

(FILE 'REGISTRY' ENTERED AT 12:04:32 ON 22 NOV 2006)

DEL HIS Y

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 8 S L2

L4 155 S L2 FUL

FILE 'CAPLUS' ENTERED AT 12:08:03 ON 22 NOV 2006

L5 3 S L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	15.79	185.14
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

STN INTERNATIONAL LOGOFF AT 12:08:50 ON 22 NOV 2006

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L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN AN 2006:1118713 CAPLUS <u>Full-text</u>
TI Preparation of diazepanes as LFA-1 inhibitors
IN Oberhauser, Berndt; Scholz, Dieter
```

PA Novartis AG, Switz.; Novartis Pharma GmbH

SO PCT Int. Appl., 60pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

GI

	PATENT NO.					KIND DATE					APPL	ICAT		DATE				
ΡI	WO 2006111371			A1 20061026			Ī	WO 2	006-1		20060419							
		W:	AE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
			ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
			ŚG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
			GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	ΚZ,	MD,	RU,	ТJ,	TM										
PRAI	PRAI GB 2005-7918					Α		2005	0419									

The title compds. I [R1 = alkyl; R2 = (un)substituted alkyl, alkenyl, alkynyl; R3 = (un)substituted aryl], e.g. useful for treating disorders or diseases mediated by LFA-1 (Leukocyte Function-Associated Antigen One), were prepared General procedures for synthesis of compds. I are given, and 65 compds. of I were prepared II showed inhibition of adhesion of LFA-1 to ICAM-1 with an IC50 value of 0.09  $\mu$ M.

IT 913357-85-4P 913358-41-5P 913358-53-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of diazepanes as LFA-1 inhibitors)

Ι

RN 913357-85-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913357-84-3 CMF C28 H31 C1 N4 O3

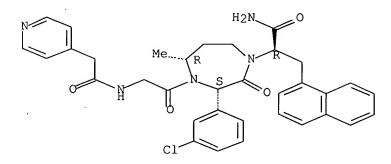
Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-41-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



RN 913358-53-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

IT 913357-86-5P 913357-87-6P 913357-88-7P 913357-89-8P 913357-90-1P 913357-91-2P

913357-92-3P 913357-93-4P 913357-94-5P 913357-96-7P 913357-98-9P 913357-99-0P 913358-01-7P 913358-03-9P 913358-04-0P 913358-05-1P 913358-07-3P 913358-09**-**5P 913358-11-9P 913358-12-0P 913358-13-1P 913358-15-3P 913358-17-5P 913358-18-6P 913358-19-7P 913358-21-1P 913358-23-3P 913358-24-4P 913358-25-5P 913358-26-6P 913358-27-7P 913358-28-8P 913358-30-2P 913358-31-3P 913358-32-4P 913358-33-5P 913358-35-7P 913358-36-8P 913358-37-9P 913358-38-0P 913358-39-1P 913358-40-4P 913358-42-6P 913358-43-7P 913358-44-8P 913358-45-9P 913358-46-0P 913358-47-1P 913358-48-2P 913358-49-3P 913358-50-6P 913358-51-7P 913358-52-8P 913358-54-0P 913358-55-1P 913358-56-2P 913358-57-3P 913358-58-4P 913358-59-5P 913358-60-8P 913358-61-9P 913358-62-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of diazepanes as LFA-1 inhibitors)

RN 913357-86-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

HC1

RN 913357-87-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

● HCl

RN 913357-88-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

#### ● HCl

RN 913357-89-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

## ● HCl \_

RN 913357-90-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

#### ● HCl

RN 913357-91-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

## ● HCl

RN 913357-92-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

# ● HCl

RN 913357-93-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913357-94-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913357-96-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913357-95-6 CMF C29 H32 C1 N5 O4

Absolute stereochemistry.

$$H_2N$$
 $Me$ 
 $R$ 
 $N$ 
 $S$ 
 $O$ 
 $C1$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913357-98-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913357-97-8 CMF C35 H42 C1 N5 O6

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913357-99-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-01-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM · 1

CRN 913358-00-6 CMF C32 H36 C1 N5 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-03-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-02-8 CMF C32 H36 C1 N5 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-04-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-05-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-07-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-06-2 CMF C37 H45 Cl N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-09-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-08-4 CMF C33 H38 C1 N5 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-11-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-10-8 CMF C33 H38 C1 N5 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-12-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-13-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-15-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-14-2 CMF C33 H38 C1 N5 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-17-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-16-4 CMF C34 H40 Cl N5 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-18-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-19-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

HCl

RN 913358-21-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-20-0 CMF C33 H39 C1 N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-23-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-22-2

CMF C33 H39 C1 N6 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 913358-24-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-25-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

HC1

RN 913358-26-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-27-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-28-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

RN 913358-30-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-29-9 CMF C30 H34 C1 N5 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-31-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

RN 913358-32-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-33-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 913358-34-6 CMF C31 H36 C1 N5 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 913358-36-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-38-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-39-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-40-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-42-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-43-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-44-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-45-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-46-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

● HCl

RN 913358-48-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-49-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-50-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 913358-51-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-52-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-54-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

RN 913358-55-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-56-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-57-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

RN 913358-58-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

● HCl

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RN 913358-59-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 913358-60-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

● HCl

RN 913358-61-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

RN 913358-62-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

● HCl

RN 913358-64-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RN 913358-66-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

App's

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L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN AN 2004:633924 CAPLUS Full-text
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DN 141:174198

TI Preparation of diazepanes as LFA inhibitors

IN Oberhauser, Berndt; Meingassner, Gottfried

PA Novartis Ag, Switz.; Novartis Pharma GmbH

SO PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

r AIN.	CNII		_													
	PATENT	KIND		DATE			APPI	LICAT	ION	DATE						
			_													
PΙ	WO 200	O 2004065382				20040805			WO 2	2004-		20040122				
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		CN, CO														
		GE, GH														
		LK, LR													•	•
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	WO 200	4-EP514		W		2004	0122									
OS	MARPAT	141:174	198													
GI																

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

The title compds. [I; R1 = alkyl; R2 = alkyl, arylalkyl, etc.; R3 = aryl], e.g. useful for treating disorders or diseases mediated by LFA-1/ICAM-1, LFA-1/ICAM-2, LFA-1/ICAM-3 or LFA-1/JAM-1 interactions, were prepared General procedures for synthesis of compds. I are given. 43 Compds. I were prepared The compound I [R1 = Me; R2 = 6-quinolinylmethyl; R3 = 3-Cl-4-FC6H3] was tested for inhibition of allergic contact dermatitis (ACD) in vivo in mice, and exhibited an inhibition of the inflammatory response by 40-50% at 0.01-10.0 mg/kg.

TT 733802-07-8P 733802-08-9P 733802-09-0P 733802-10-3P 733802-11-4P 733802-13-6P 733802-14-7P 733802-15-8P 733802-16-9P 733802-17-0P 733802-19-2P 733802-20-5P 733802-21-6P 733802-22-7P 733802-23-8P 733802-24-9P 733802-25-0P 733802-26-1P 733802-30-7P 733802-31-8P 733802-32-9P 733802-33-0P 733802-34-1P 733802-35-2P

733802-37-4P 733802-38-5P 733802-40-9P

733802-41-0P 733802-42-1P 733802-44-3P

733802-45-4P 733802-47-6P 733802-48-7P

733802-49-8P 733802-50-1P 733802-51-2P

733802-52-3P 733802-54-5P 733802-55-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of diazepanes as LFA inhibitors)

RN 733802-07-8 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-08-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 733802-09-0 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(4-fluorophenyl)hexahydro-5-methyl- $\alpha$ - (1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-10-3 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(2-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-11-4 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-bromophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & Br & O & CH_2 & O \\ & O & CH_2 & O & CH_2 & O \\ & H_2N-C-CH-N & N-C-CH_2 & O \\ & Me & . & & \\ \end{array}$$

RN 733802-13-6 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-[1,1'-biphenyl]-3-ylhexahydro-5-methyl-  $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-12-5 CMF C42 H38 N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 733802-14-7 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-15-8 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3,5-dichlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-16-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-[4-chloro-3-(trifluoromethyl)phenyl]hexahy dro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)-(9CI) (CA INDEX NAME)

RN 733802-17-0 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chloro-4-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & F \\ O & CH2 \\ H2N-C-CH-N & N-C-CH2 \\ \hline \\ Me \end{array}$$

RN 733802-19-2 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)-3-[2-(trifluoromethyl)phenyl]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-18-1 CMF C37 H33 F3 N4 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 733802-20-5 CAPLUS

CN lH-1,4-Diazepine-1-acetamide, 3-(3,4-difluorophenyl)hexahydro-5-methyl-  $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-21-6 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-cyanophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & \circ & & \\ \text{H}_2\text{N}-\text{C}-\text{CH}-\text{N} & & \\ & & & \\ & & & \\ \text{Me} & & \\ \end{array}$$

RN 733802-22-7 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-[3-(5-pyrimidinyl)phenyl]-4-(6-quinolinylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-23-8 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-(6-quinolinylacetyl)-3-[3-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 733802-24-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)-3-(3-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

RN 733802-25-0 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

RN 733802-26-1 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-

(9CI) (CA INDEX NAME)

RN 733802-27-2 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)-3-(3-chloro-4-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & F \\ \hline \\ H_2N-C-CH-N & N-C-CH_2 \\ \hline \\ CH_2 & Me \end{array}$$

RN 733802-28-3 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)-3-(3-cyanophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

RN 733802-29-4 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-(1,3-benzodioxol-5-ylacetyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-[3-(trifluoromethoxy)phenyl]-(9CI) (CA INDEX NAME)

RN 733802-30-7 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -

(1-naphthalenylmethyl)-2-oxo-4-(phenylacetyl)- (9CI) (CA INDEX NAME)

RN 733802-31-8 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-fluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-[[3-(trifluoromethyl)phenyl]acetyl]- (9CI) (CA INDEX NAME)

RN 733802-32-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-[1,1'-biphenyl]-4-ylhexahydro-5-methyl-  $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-[(2,3,6-trichlorophenyl)acetyl]- (9CI) (CA INDEX NAME)

RN 733802-33-0 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[(4-cyanophenyl)acetyl]-3-(3,4-difluorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

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RN 733802-34-1 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)-4-[(4-cyanophenyl)acetyl]hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

RN 733802-35-2 CAPLUS

CN lH-1,4-Diazepine-1-acetamide, 4-[(4-aminophenyl)acetyl]-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 733802-37-4 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[(4-aminophenyl)acetyl]hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-36-3 CMF C34 H33 F3 N4 O3

PAGE 2-A

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 733802-38-5 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[[4-(dimethylamino)phenyl]acetyl]hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 733802-40-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[(3-aminophenyl)acetyl]-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-39-6 CMF C33 H33 C1 N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 733802-41-0 CAPLUS

CN Butanoic acid, 4-[[4-[2-[4-[2-amino-1-(1-naphthalenylmethyl)-2-oxoethyl]hexahydro-7-methyl-3-oxo-2-[3-(trifluoromethyl)phenyl]-1H-1,4-diazepin-1-yl]-2-oxoethyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 733802-42-1 CAPLUS

CN Butanoic acid, 4-[[4-[2-[4-[2-amino-1-(1-naphthalenylmethyl)-2-oxoethyl]-2-(3-chlorophenyl)hexahydro-7-methyl-3-oxo-1H-1,4-diazepin-1-yl]-2-oxoethyl]phenyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 733802-44-3 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[[4-[(aminoacetyl)amino]phenyl]acetyl]-3- (3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-43-2 CMF C35 H36 C1 N5 O4

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 733802-45-4 CAPLUS

CN lH-1,4-Diazepine-1-acetamide, 4-[[3-[(aminoacetyl)amino]phenyl]acetyl]-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 733802-47-6 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[[4-[(3-amino-1-oxopropyl)amino]phenyl]acetyl]-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 733802-46-5 CMF C36 H38 C1 N5 O4

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CRN 76-05-1 CMF C2 H F3 O2

RN 733802-48-7 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-4-[[4-[(1-oxo-2-propenyl)amino]phenyl]acetyl]-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 733802-49-8 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-5-methyl-4-[[4-[[4-(4-morpholinyl)-1,4-dioxobutyl]amino]phenyl]acetyl]- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

PAGE 2-A

RN 733802-50-1 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)-4-[[4-[[1,4-dioxo-4-(1-piperazinyl)butyl]amino]phenyl]acetyl]hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo- (9CI) (CA INDEX NAME)

RN 733802-51-2 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-4-[(2-methoxyphenyl)acetyl]-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo- (9CI) (CA INDEX NAME)

RN 733802-52-3 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 3-(3-chlorophenyl)hexahydro-4-[(4-methoxyphenyl)acetyl]-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo- (9CI) (CA INDEX NAME)

RN 733802-54-5 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[(3-chloro-4-methoxyphenyl)acetyl]-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

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RN 733802-55-6 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-acetyl-3-(3-chlorophenyl)hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-(9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
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AN 2001:283944 CAPLUS Full-text

DN 134:311434

TI Preparation of naphthylalaninyldiazepinones and related compounds for treating disorders or diseases mediated by LFA-1/ICAM-1, -ICAM-2 or -ICAM-3 interactions.

IN Albert, Rainer; Ehrhardt, Claus; Hommel, Ulrich; Kallen, Joerg;
 Meingassner, Josef Gottfried; Roche, Didier; Wattanasin, Sompong;
 Weitz-Schmidt, Gabriele; Welzenbach, Karl

PA Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.

SO PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.					KIND		DATE		APPLICATION NO.						DATE		
ΡI	WO 2001027102				A1		20010419		WO 2000-EP10025					20001011				
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Title compds. [I; n = 1-3; R1 = H, alkyl, aryl, aralkyl; Y = alkylene, alkenylene, CONH, CO2, etc.; R2 = (substituted) aryl, heteroaryl; R3 = amino acid side chain; R4 = (substituted) biphenylyl, PhCH2, hydroxybenzyl,  $\beta$ -naphthylmethyl, tetrahydro- $\beta$ -naphthylmethyl, indolylmethyl; X = cyano, amino, OH, alkoxy, etc.], were prepared Thus, (S)-2-[(3S,5R)-3-isobutyl-5-methyl-2-oxo-1,4-diazepan-1-yl]-3-(naphthalen-2-yl)propionamide, 6-quinolylacetic acid, (Me2CH)2NEt, and EADC were stirred 16 h in CH2Cl2 to give (S)-2-[(3S,5R)-3-isobutyl-5-methyl-2-oxo-4- (quinolin-6-ylacetyl)-1,4-diazepan-1-

y1]-3-(naphthalen-2-y1)propionamide. The latter inhibited adhesion of LFA-1 to ICAM-1 with IC50 =  $0.44~\mu M$ .

IT 334941-36-5P 334941-49-0P 334941-54-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of naphthylalaninyldiazepinones and related compds. for treating disorders or diseases mediated by LFA-1/ICAM-1, -ICAM-2 or -ICAM-3 interactions)

RN 334941-36-5 CAPLUS

CN lH-1,4-Diazepine-1-acetamide, hexahydro-5-methyl- $\alpha$ -(2-naphthalenylmethyl)-2-oxo-3-phenyl-4-(6-quinolinylacetyl)-, ( $\alpha$ R,3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 334941-49-0 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, hexahydro-5-methyl-4-(2-naphthalenylacetyl)- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-phenyl- (9CI) (CA INDEX NAME)

RN 334941-54-7 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, 4-[(3,4-dichlorophenyl)acetyl]hexahydro-5-methyl- $\alpha$ -(1-naphthalenylmethyl)-2-oxo-3-phenyl- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT